COMPUTER-AIDED PROCESS ENGINEERING (CAPE) : EDUCATION AND PRACTICE

By

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Abstracts

In this paper, the important roles of computer-aided tools in solving problems in process engineering are highlighted. Few research which have been done in the area of CAPE are focused on and results from these research is reported. The future direction of CAPE is also presented.

1. Introduction

In the last few years, the growing complexities of chemical plants/processes and also the competitiveness in the chemicals market has made the utilization of computer becoming more significant. The computer has been used extensively in designing new plants/processes, retrofitting existing plants, training operators and engineers, and many others.

With the rapid pace of the development of computer's capabilities (it was reported that these capabilities have increased by two orders of magnitude per decade, [Stadtherr etc.,1993]), many difficult tasks have been made easy especially in simulation activities. Simulation, which can be applied at all stage of process life, can ensure increasing profits and productivity, safe operation, and more important, money and time savings through the reduction of pilot plant trials.

The education and practice in process engineering were significantly influenced by the computerization. We will probe further into how these changes took place and it's direction in the future. First, let us look at the definition of CAPE itself. Process Engineering is defined as "the application of systems concepts and methodologies to the design and operation of chemical processes" (Westerberg,1991). Therefore, we could define CAPE as the application of systems concepts and methodologies to the design and operation of chemical processes aided by computerization. Figure 1 shows the scopes and applications generally covered by CAPE.

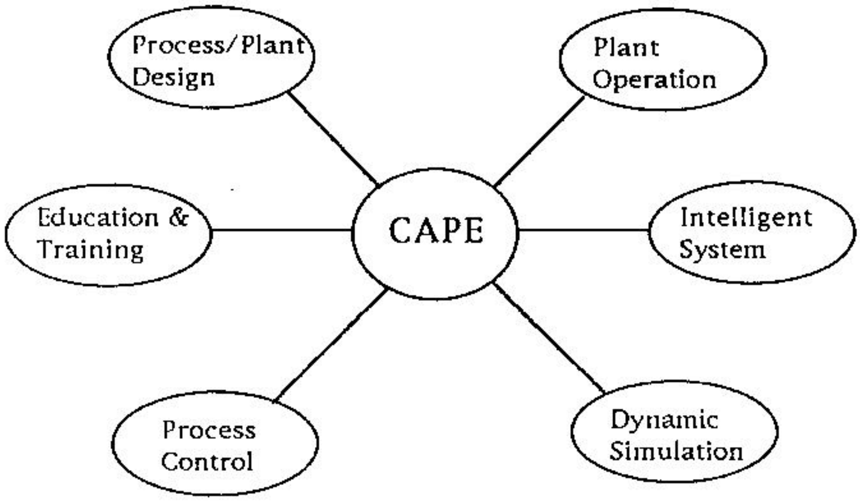


Figure 1 Scopes of CAPE

Since the areas under CAPE are quite large, our group, the Process System Engineering (PSE) in the Department of Chemical Engineering, FKKKSA, are trying to concentrate on a few aspects of these areas. Under the program CAPE, there are few research projects are currently being carried out and also planned. Table 1 shows list of projects :

Table 1 List of Projects under the Program CAPE

no.	Project
1.	Modeling, Simulation and Control of Liquid Flow and Level System
2.	Development of Heated Tank Control System
3.	Development of Batch Reactor/Fermenter Control System
4.	Dynamic Simulation of Batch/Continuous Distillation Process
5.	Guidance System for the Startup Operation of Batch Distillation
6.	Development of Flash Dryer Control System
7.	Application of Multimedia in Developing Chemical Engineering Education Software Package
8.	Studies on the Interaction between Design and Control
9	Process Control Software for Training in Education and Industry Sectors
10.	Software Development for Process/Plant Integration

Results for three of the above projects will be discussed in the following section.

2. Examples of Research Projects under CAPE

2.1 Flow Control System

2.1.1 Introduction

Flow control, a common control system in chemical process plants, is used to control the flow rate of a gas or liquid stream. In this study, an electronic flow control system is modeled, simulated and experimentally controlled to fully understand the system. Learning from the system is important because flow control is present in almost all other chemical process control systems. This part of the paper will highlight some results obtained in studying the flow control system, which is the comparison of responses obtained from different tuning methods and also between different types of feedback controllers. Results for tuning parameters calculated using the Integral of the Time-weighted Absolute Error (ITAE) which uses the process reaction curve and the continuous cycling Ziegler-Nichols method are discussed.

2.1.2 System Description

The flow control system, manufactured by Cussons of England, originally came with stand-alone controllers and chart-recorders. However, the system is now interfaced to a personal computer that acts as a controller. GENESIS, the control software used, provides a complete environment for creating and running industrial process control schemes and data acquisition. For the flow control system, a PID controller equation is applied.

Fig. 2 illustrates the schematic diagram of the control system. A centrifugal pump is employed to pump around water from the storage tank. The orifice plate and the flow transducer (with square root extractor) measures the flow rate and sends a 0 to 10 volt signal to the controller. The flow meter shown in Figure 2 is a rotameter which had been calibrated to give readings in liters/hour of water. The flow sensor sends a signal of the measured variable to the controller (in this case, the computer) and after some calculations, the controller sends back a signal instructing the control valve the action it should take. The suitability of the controller action depends on the controller tuning parameters entered into the computer. Fig. 3 shows the "control panel" display for the flow control system where the tuning parameters for the PID controller (controller gain, Kc, reset time, ti and derivative time, td), are entered. Turning on the pump from the panel activates data logging. Also, real-time plots and plots of different responses to different tuning parameters that has been performed can be observed from the computer by opening historian files.

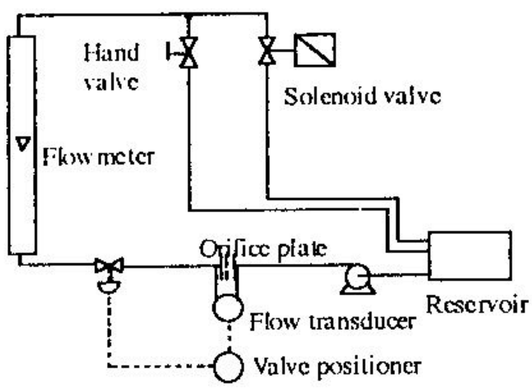


Fig. 2 Flow control system

2.1.3 Procedure

The control valve characteristic must initially be obtained to determine a linear region of operation. This was performed by recording the flowrate at several percentages of valve opening while the controller is in manual .

With the operating region identified, an open-loop step change in the valve opening was executed. From the open-loop step response, a first-order plus dead-time model was estimated. Upon attaining the model, the tuning parameters for the ITAE tuning criterion were calculated.

For the Ziegler-Nichols method, the integral and derivative mode was first eliminated to find the ultimate gain and the ultimate period. Setting the controller gain, Kc, to a small value with the controller on automatic, a set point change was performed. The value of Kc was slowly increased until sustained oscillations occurred. The continuous oscillations can be observed from the real-time data-logging historian file in the computer. At this point, the value of the controller gain is the ultimate gain and the period of oscillations of the response is the ultimate period. The tuning parameters can then be calculated using the Ziegler-Nichols tuning relations.

To test the tuning parameters, the controller was set to automatic and an initial set point and the controller settings were entered. When the flowrate was approximately constant, a new set point was entered and the data recorded in a historian file.

2.1.4 Results

From the valve characteristic curve, shown in Fig. 4, the operating region was determined to be from 50% to 100% opening which corresponds to a flow rate of 146 to 560 liters/hour. This is because about 96% of the flow rate that can be controlled by the valve falls within this domain.

Applying the 28%-63% method on the step response, the estimated first-order plus dead-time model, in Laplace transform, is:

$$G(s) = \exp(-3.3s) / (5.7s + 1)$$

where the dead-time and time-constant units are in seconds.

Table 2 shows the tuning parameters found using the ITAE tuning criterion calculated from this model. The settings found using the Ziegler-Nichols tuning technique is also stated in the table.

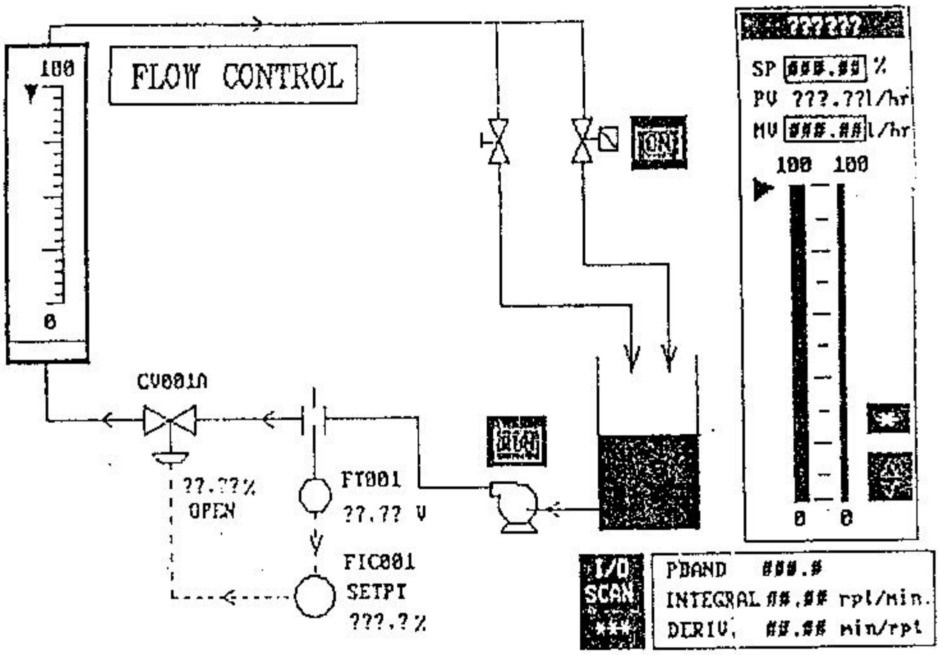


Figure 3. Flow Control Screen

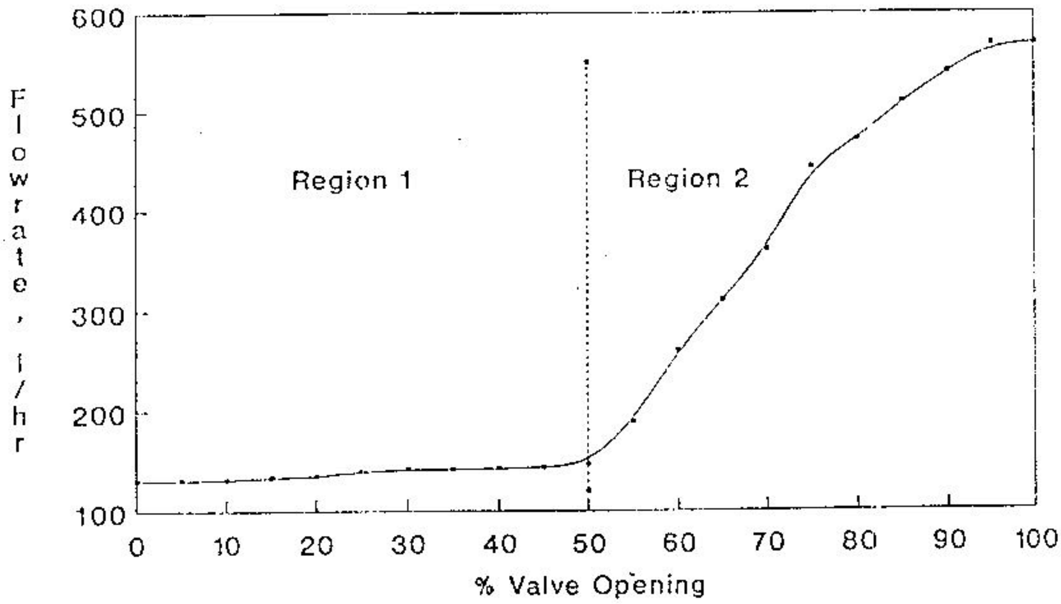


Figure 4 Control Valve Characteristic

Table 2 Tuning parameters

Method	Controller	Kc	ti	td
ITAE	PI	0.97	6.10	-
	PID	1.54	8.02	1.06
Ziegler - Nichols	P	1.48	-	-
	PI	1.33	10.83	-
	PID	1.77	6.50	1.63

In testing the controller settings, a set point change from 300 to 400 liters per hour was performed for all cases. The response for a set point change using the P controller is shown in Fig. 5. The ITAE criterion has no controller settings for the P controller. Fig. 6 and Fig. 7 illustrate the response for a set point change using the PI and PID controllers respectively.

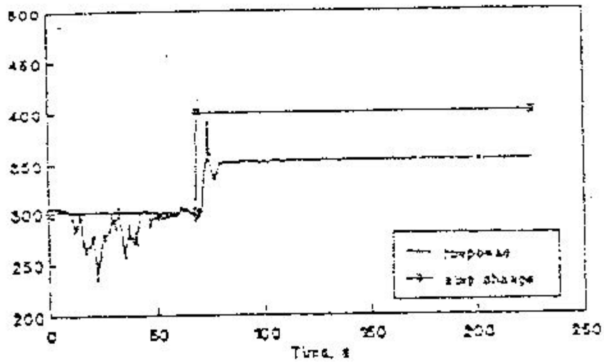


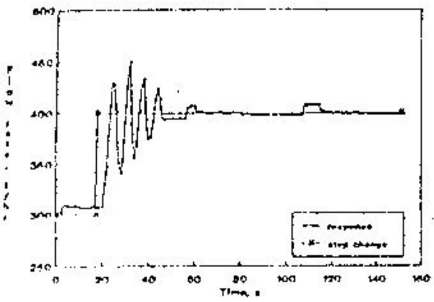
Figure 5. Response of a Set Point Change With a P Controller

2.1.5 Discussions

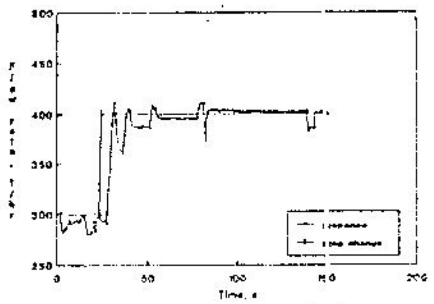
Of the two tuning methods, the parameters calculated using the ITAE criterion gave the best response for both the PI and PID controllers. Although the criterion gave conservative settings compared to the Ziegler-Nichols method, the response acquired using both controllers had little fluctuations and small settling times.

The response of the set point change obtained with the P controller conformed with a known fact that using a P controller will always result in offsets. True to the theory, the addition of the I (integral) mode eliminates offsets, as shown in Fig. 6 and Fig. 7.

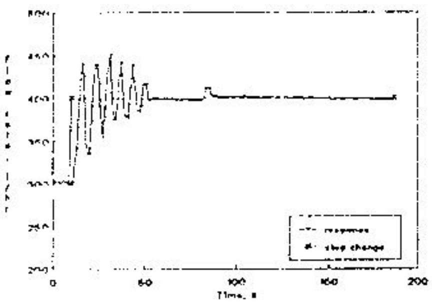
Of the three controllers, the PI controller was found to be the most suitable controller. The responses obtained using both methods were stable and had no



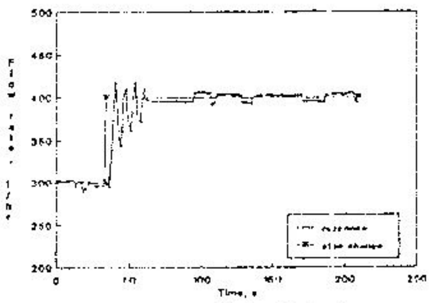
IAE Servo Mode Tuning Criteria



ITAE Servo Mode Tuning Criteria

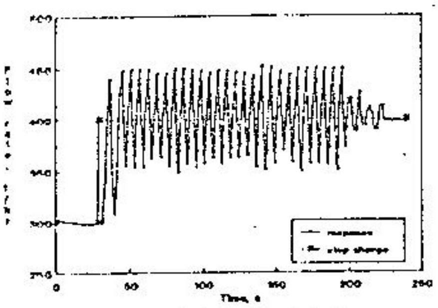


Trial & Error Tuning Method

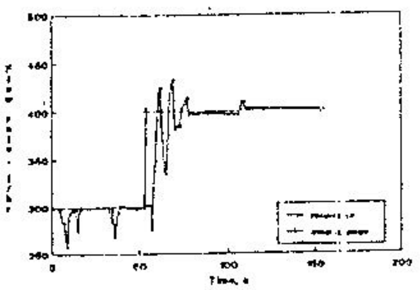


Ziegler-Nichols Tuning Method

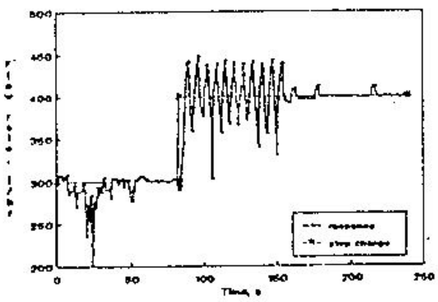
Figure 6 Responses of a Set Point Change with a PI Controller



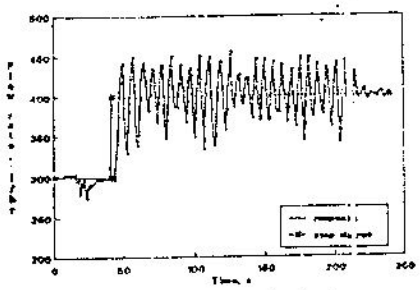
IAE Servo Mode Tuning Criteria



ITAE Servo Modo Tuning Criteria



Trial & Error Tuning Method



Ziegler-Nichols Tuning Method

Figure 7 Responses of a Set Point Change with a PID Co.troller steady-state offset. Addition of the derivative mode (resulting in a PID controller) seems to destabilize the system. Observe also that the anticipatory action of the derivative mode was greatly affected by fluctuations in flow rate of not more than ± 10 liters/hour caused by the pump. Also, as flow systems are fast (small time constants and dead-times), the anticipatory function of the derivative mode is not really necessary. This can be seen from responses obtained using PI and PID controllers with parameters from the ITAE criterion where both responses have similar fluctuations and settling times. The results, therefore, show that having an additional controller mode is not always better.

2.2 Batch Reactor/Fermenter Control System

2.2.1 Introduction

Initial stages of research on temperature and pH control using a batch reactor/fermenter control system is presented. pH control is notorious for its difficulty because of the nonlinear nature of the titration curve. There is therefore tremendous potential for research. On the other hand, temperature control is fairly easier compared to pH control. Nevertheless, temperature control is just as important to understand and explore because of its common occurrence in industry. Since the system has just been commissioned, the experiments were mainly conducted as initial tests for the control and data logging system. However, the results obtained from the experiments performed were surprisingly encouraging.

2.2.2 System and Process Description

Figure 8 illustrates a schematic diagram of the fermenter/batch reactor control system. The reactor is a two-liter jacketed glass vessel. A personal computer with an 80386 microprocessor with math co-processor serves as a controller and data logger. The water bath heats up the heating fluid while a pump is employed for circulation. A temperature sensor (Pt 100) measures the temperature in the reactor and power to the heating coil in the water bath is manipulated to achieve temperature control. For pH control, a pH sensor is used to gauge the pH in the reactor. Dosing from two peristaltic pumps (one for the acid solution and one for the base solution) are manipulated.

The process, which is the anaerobic conversion of glucose to ethanol using yeast immobilized alginic acid, is shown in Figure 9. The immobilized yeast is packed in a glass tube (about 2 cm. in diameter). Referring to the figure, a pump circulates glucose and ethanol that had been formed from the glass vessel to the packed bed reactor and back to the vessel. In this process, the reaction actually occurs in the glass tube, where without oxygen, the yeast produces an enzyme to convert glucose to ethanol. For the experiment, the desired temperature and pH are 35°C and 5.5 respectively. The acid and base solutions used for pH control are hydrochloric acid (HCl) and sodium hydroxide ($NaOH$) respectively. The reaction is chosen because without proper pH control, the reactants will become highly acidic, killing off the yeast.

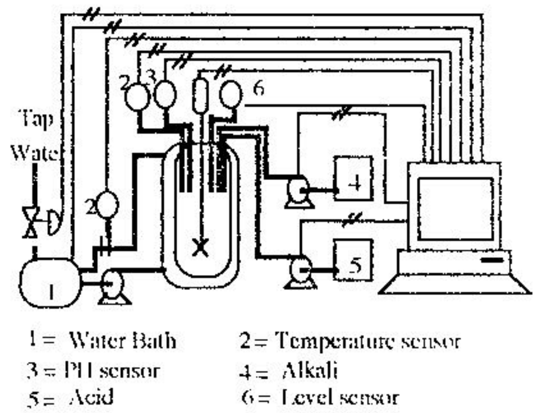


Figure 8. Batch reactor/fermenter control system

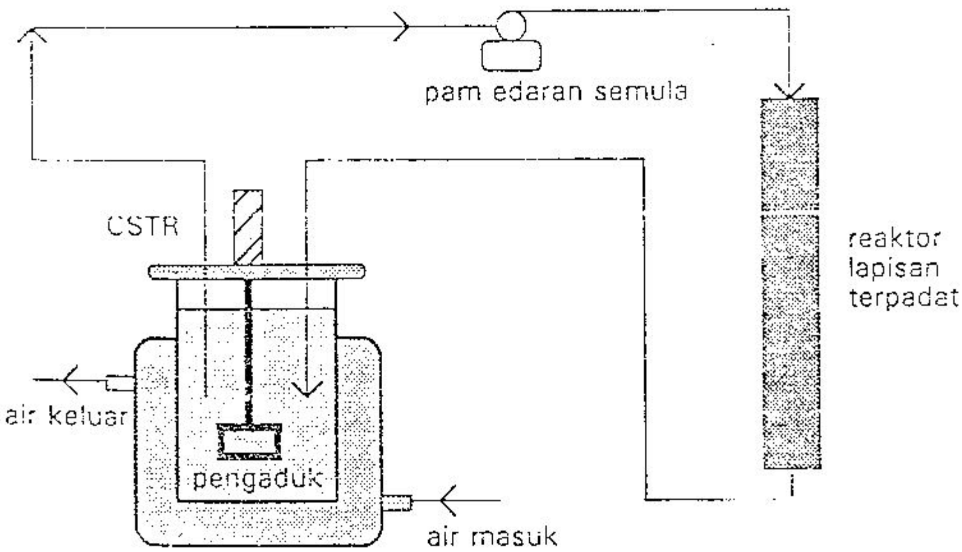


Figure 9 The process using yeast immobilized alginic acid

Consequently, conversion will stop. Proper control of temperature is also needed to ensure optimal conversion.

2.2.3 Procedure

The experimental runs can be divided into two categories: "dry" runs, which are runs made without the reaction, and "wet" runs, which are runs made with the reaction. Dry runs are essential to really understand the control systems as they are performed without the complication contributed by the reaction. Tuning parameters for the wet runs were also obtained from the dry runs. The tuning parameters for temperature control were calculated using the Integral of the Absolute value of the Error (IAE) tuning criterion based on the first order plus dead-time model of the temperature step response. For pH control, the tuning parameters were calculated using the Ziegler-Nichols tuning method.

Two wet runs were made: the first without controllers (open-loop), while the second was accomplished with controllers (closed-loop). For both runs, before executing the experiment, the immobilized yeast packing in the form of beads is first prepared by slowly dripping a solution of yeast, yeast extract and alginic acid from a syringe into a 1 M calcium chloride solution. Detailed procedure is reported by Choo (1993). In the open-loop run, the reactants were circulated through the packed bed without and temperature or pH control. However, the process temperature, pH and glucose content were monitored throughout the experiment. In the close-loop run, the IAE tuning parameter in servo mode were used to control the temperature at start-up. Once start-up has been completed, the tuning parameters were changed to those calculated in regulatory mode. For pH control, the tuning parameters obtained from the dry run were applied.

2.2.4 Results and Discussions

The characteristic curve for the heater in the water bath is shown in Figure 10. An open-loop dry run step change in the heater power from 400 watt to 600 watt was executed. This temperature region was chosen because this is approximately where the process will be operating. The estimated FOPDT model calculated is

$$G(s) = (0.66\, e^{-465s})/(4920s + 1)$$

where the dead-time and time constants are given in seconds. The IAE tuning parameters calculated for a PID controller are: Kc = 19.09, ti = 957.44 seconds and td = 162.23 in regulatory mode and Kc = 12.78, ti = 6760.9 seconds and td = 198.22 in servo mode.

Figure 11 shows the titration curve between 0.1M NaOH and 0.1M HCl. A set point at pH 5.5 would be difficult to control because its location on the steep part of the curve. This highly non-linear situation causes the system to have an uneven process gain when equal concentration of acid and base solutions are utilized -- a low gain going to the acidic side (small change in pH for a fixed volume of acid) and a high gain going to the basic side (large change in pH for a fixed volume of base). In an effort to counter this lopsided gain

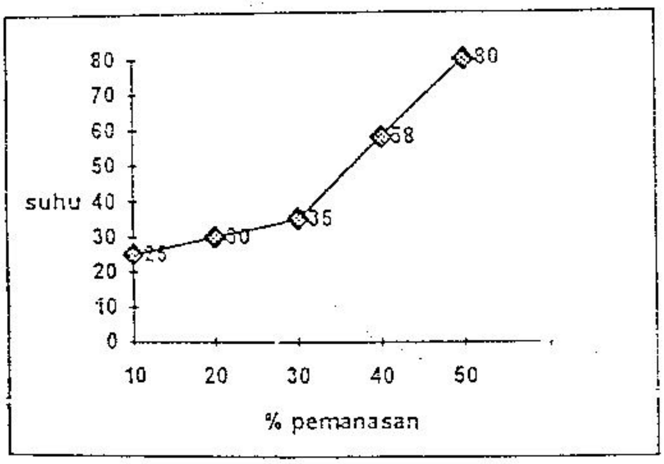


Figure 10 Characteristic curve of the heater

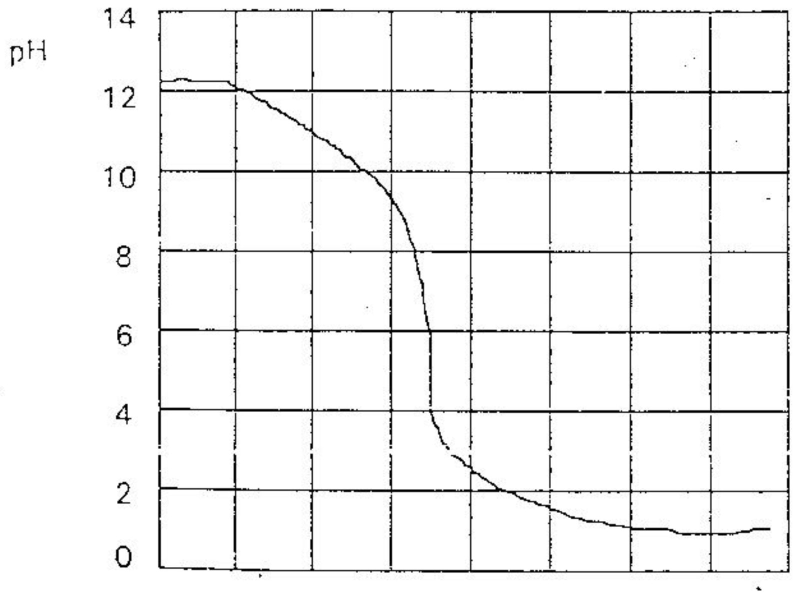


Figure 11 Titration curve

effect, a more dilute base solution was used. A less concentrated base solution compared to the acid concentration would allow a higher volume of base to be pumped in to attain a fixed change in pH. Consequently, the process gain would be somewhat evened out. Utilizing this idea, Kc, ti and td found using the Ziegler-Nichols method are 58.82, 5 and 1.25 respectively.

The open-loop wet run were performed for about 13.5 hours. Temperature and pH for the first six hours can be seen in Figure 12. The temperature of the process are observed to be closely following the room temperature, while the pH slowly became more acidic, until it leveled off at 3.1. Figure 13 shows the glucose content in the reactant and product solution. From the figure, the glucose content is still very high even after 50,000 seconds (i.e.. 13.9 hours). This indicates that the conversion of glucose to ethanol is very low.

Figure 14 illustrates the temperature and pH response of the final closed-loop wet run. Referring to Figure , there is about a 12% overshoot with a decay ratio of approximately 5%, causing the temperature to rapidly settle at the set point. The pH response is equally favorable. The controller was able to keep the pH at the set point of 5.5, with only minor fluctuations. Glucose concentration throughout the experiment is given in Figure 15. The glucose conversion calculated for the open-loop and closed-loop at seven hours are 22.31 mg/dL.hr and 49.14 mg/dL.hr respectively. Hence, the closed-loop conversion is twice the open-loop conversion.

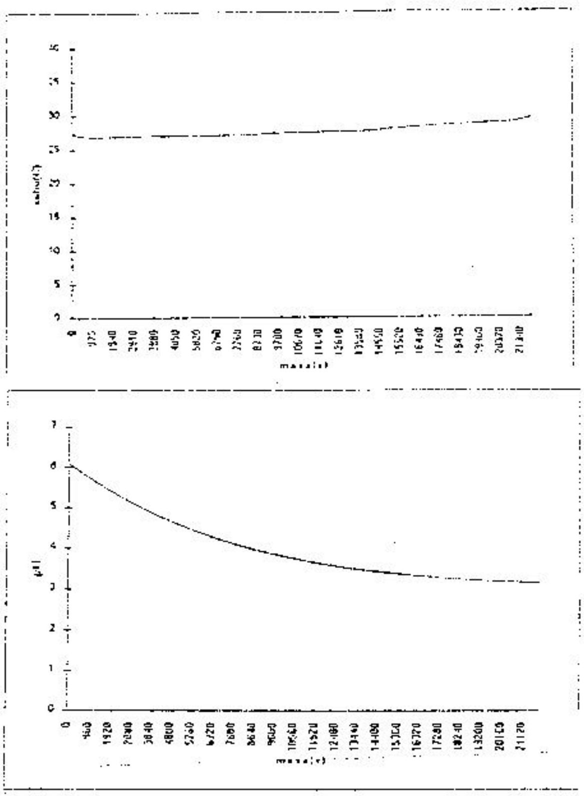


Figure 12 Temperature and pH response (open-loop)

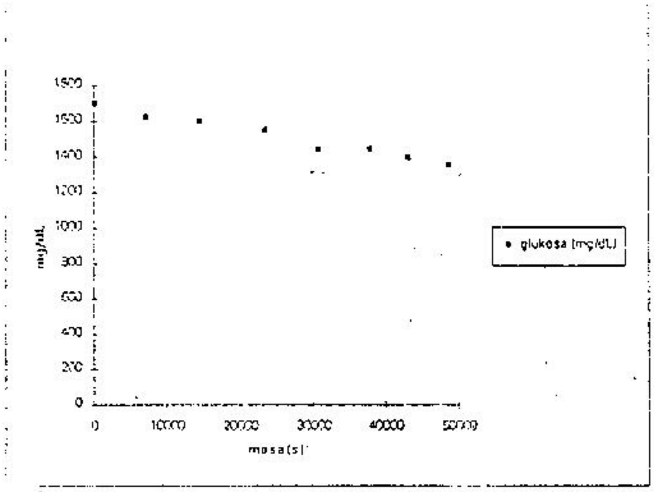


Figure 13 Glucose content in reactant and product

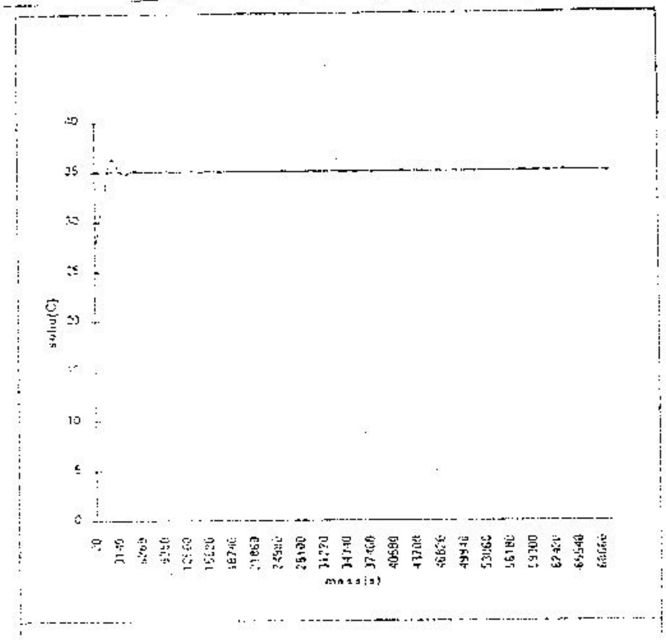


Figure 14 Temperature response (closed-loop)

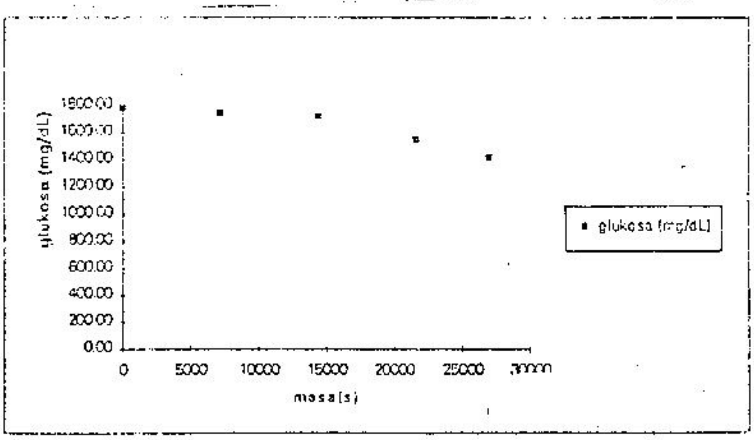


Figure 15 Glucose conversion (closed-loop)

2.3 Multimedia in Chemical Engineering Education

2.3.1 Introduction

Multimedia is a presentation of information through more than one presentation media such as text, sounds, musics, graphics, image, animation and video. These combinations of media will produce interesting effects to the user. In general, the basic usage of multimedia can be divided into four categories i.e. live presentation, desktop video publishing and production, interactive application and desktop, and animation and visualization. Recently, multimedia has emerge as one of the most promising and exciting fields that can be applied in many sectors such as business, industry and academic.

One of the powerful application of multimedia is in the Computer Aided Instructions (CAI). The application of multimedia in CAI can enhance the effectiveness of learning by making the process of learning more interesting and interactive. It is now being used extensively for learning and training purposes in many industries such as ICI (Shaw, 1984), Panasonic (Charles, 1983) and others. Among the popular multimedia softwares are Authorware and Micromind Director.

In this particular work, the application of multimedia in Chemical Engineering Education is highlighted. At the moment, the concentration is given to the learning of unit operations such as distillation, absorption, evaporator and others.

2.3.2 Example : Lessons on Multiple Effect Evaporator

In one section of the project, we decided to apply multimedia in teaching multiple-effect evaporator. The objective of the research is to introduce the concept of evaporation and to expose the users on different configuration of evaporators, and it's calculations.

In this work, for the hardware, we used Macintosh Computer, scanner and recorder. For developing the systematic teaching of evaporator concepts, Authorware was used as the media software.

This package of multi-effect evaporators consist of 6 sections :

1) Review of Evaporation Process
2) Advantages of Multi-effect Evaporators
3) Types of Configuration
4) Vapor Compression
5) Calculation Steps of Multi-effect Evaporator
6) Quiz

In the beginning, combinations of graphics, animation and sounds will be used to present the topics of multi-effect evaporator. Then, the user will be asked to enter his name. By referring the user's name in it's presentation, the program will be guiding the user through different sections above. The user will be given choices to select for all the sections. Figure 16 to 19 shows few of the screens that appears on the packages.

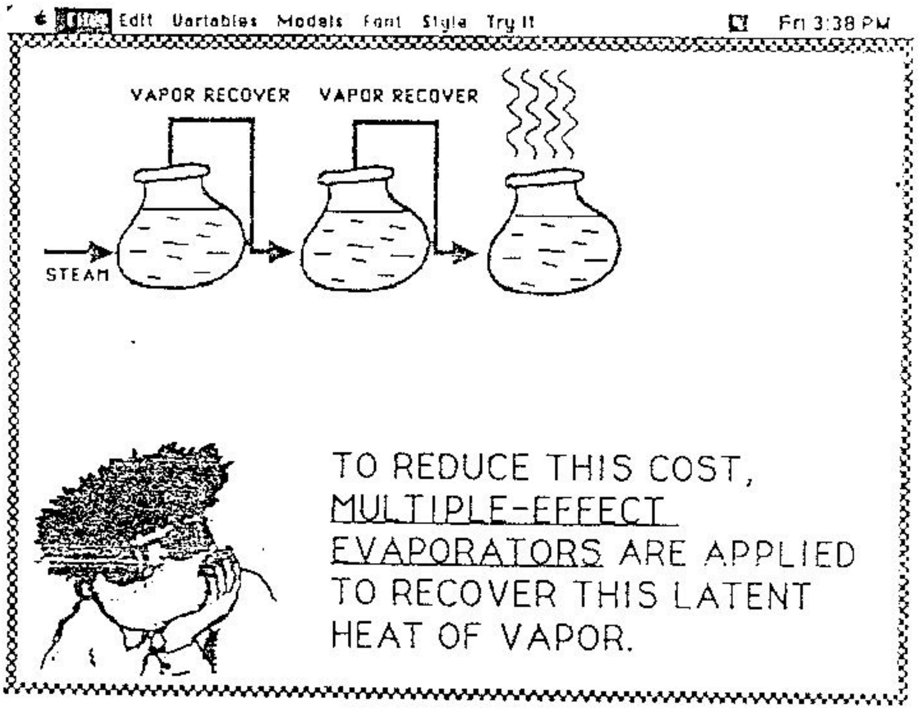


Figure 16 Example appears on the screen

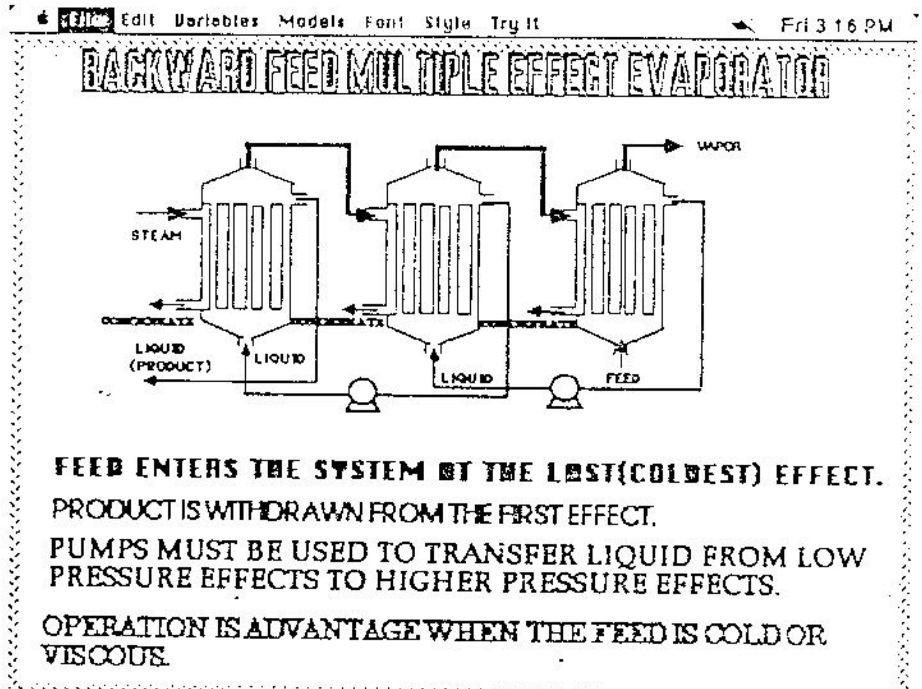


Figure 17 Example appears on the screen

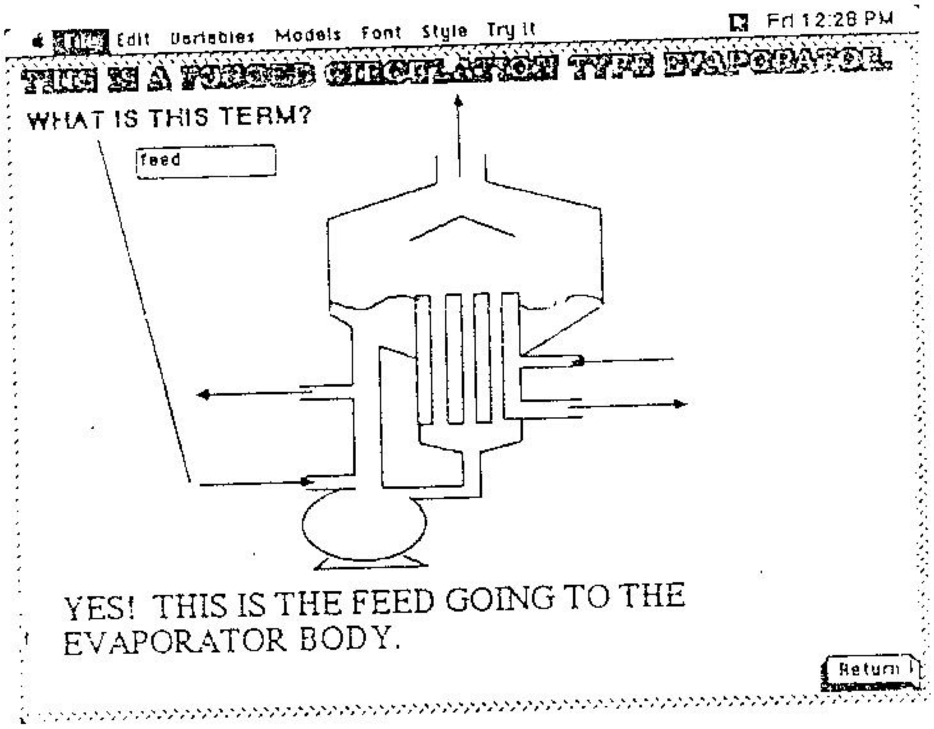


Figure 18 Example appears on the screen

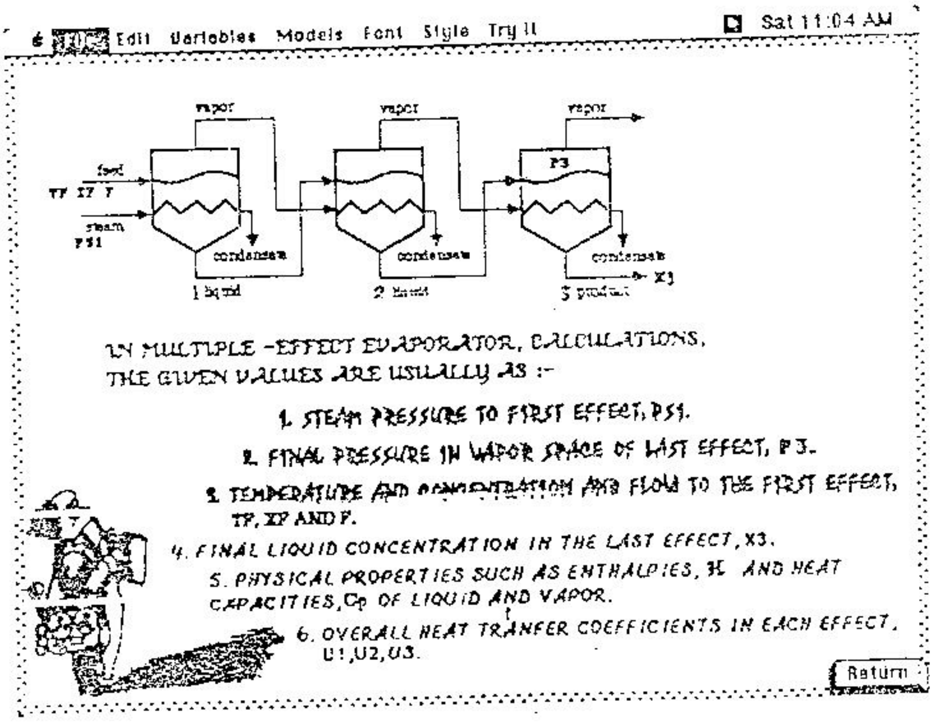


Figure 19 Example appears on the screen

2.3.3 Conclusions

At the moment, the initial work of producing an educational software package for chemical engineering has been carried out. From the work on the multi-effect evaporator, it could be said that it has been successful in fulfilling the requirement as multimedia package as the combinations of all the medias have been utilized. By presenting the aspects of multi-effect evaporators in more interesting and interactive ways, it is hope that the learning process will be more exciting and attractive for the students.

Many works have to be carried out in the future especially in upgrading the quality of the package to meet the professional standard. There is also problems in the size of the memory of the package and it can be solved by using CD ROM.

3. Future Research Direction

The question now, towards which direction of CAPE is going?. In short, it could be summarized that the main aim of all the projects in CAPE is to utilize computers in efficient manner to design, operate and control chemical process so that the plant performance could be improved. These will include activities such as modeling and simulation of the processes; training and retraining of operators and engineers using good quality education and training simulator; and others. Therefore, in the future, we foresee of integrating all the results from the research projects in developing a complete and powerful methodologies to design, operate and control the entire chemical plant. We hope to apply the knowledge gained, to the operation of several pilot plants in the Department of Chemical Engineering. One of the pilot plants will be the one that will be built in Skudai (mostly for continuous process) and the other will be "the Pipeless Batch Plant" which is now being studied and designed. In addition, the research on the aspects of education and training using multimedia will be incorporated into courses organized by the Dept. of Chemical Engineering such as CENCE (Chemical Engineering for Non-Chemical Engineers) and others.

4. Conclusions

Looking at the future direction of the research in CAPE, we believe that the potential of applying CAPE is great. CAPE can be used to enhance learning and training. In addition, the improvement of plant performance can be done optimally using computer through simulations.

Acknowledgment

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